

# GRANULAR FLUIDS

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## I. DEFINITION OF THE SUBJECT AND ITS IMPORTANCE

The terminology granular matter refers to systems with a large number of hard objects (grains) of mesoscopic size ranging from millimeters to meters. Geological examples include desert sand and the rocks of a landslide. But the scope of such systems is much broader, including powders and snow, edible products such a seeds and salt, medical products like pills, and extraterrestrial systems such as the surface regolith of Mars and the rings of Saturn. The importance of a fundamental understanding for granular matter properties can

hardly be overestimated. Practical issues of current concern range from disaster mitigation of avalanches and explosions of grain silos to immense economic consequences within the pharmaceutical industry. In addition, they are of academic and conceptual importance as well as examples of systems far from equilibrium.

Under many conditions of interest, granular matter flows like a normal fluid [1]. In the latter case such flows are accurately described by the equations of hydrodynamics. Attention is focused here on the possibility for a corresponding hydrodynamic description of granular flows. The tools of nonequilibrium statistical mechanics [3], developed over the past fifty years for fluids composed of atoms and molecules [4, 5], are applied here to a system of grains for a fundamental approach to both qualitative questions and practical quantitative predictions. Applications of basic atomic physics principles to granular fluids have accelerated during the past decade, starting with an emphasis on molecular dynamics (MD) simulations [6] and kinetic theory [7, 8], and more recently with the theoretical methods of the type described here [9, 10, 11, 12, 13, 14].

## II. INTRODUCTION

To start with the familiar, consider a jar of vitamin pills, mustard seeds, or peanuts. Remove the lid and pour them into a bowl, observing that the "flow", or their collective motion, has some similarity to that of a normal fluid such as water. The collective motion in both cases is the consequence of collisions among their constituents, grains or atoms, and their large number. It is tempting to make the correspondence of grains to atoms in considering the similarities of flows in these two types of fluids. The objective here is to explore in formal detail the extent to which that correspondence is conceptually and quantitatively justified. An important prerequisite is the integrity of the grains during their motion. Each grain is comprised of a large number of atoms or molecules. Integrity refers to their retention of mass and shape following interactions with other grains or with their environment. As such, the grains behave as "particles" whose detailed internal structure is not essential to their description, which is captured instead by a few parameters describing their shape, mass, and collisional properties with other grains. However, an important consequence of this underlying molecular structure is a redistribution of translational kinetic energy of the grains and internal energy of the constituent molecules. At the mesoscopic

level this appears as an energy loss on collisions between pairs of grains. This is a central feature of granular fluids differentiating them from atomic fluids: the inelasticity of granular pair collisions.

Granular matter occurs in two classes of states, compact and activated [15]. In the first case, the grains form a static packed configuration within the container due to the effects of gravity on their relatively large mass and their inelastic collisions. Any initial motion is quickly dissipated and their kinetic energy becomes negligible relative to the gravitational potential energy. Important questions arise about the possible and probable packing configurations that determine the stresses within the system and the distribution of forces on the container. For example, chains of particles in contact can occur as arches to support matter above them while reducing their force on the matter below. There is an intense interest in the study of such states, generically referred to as contact mechanics.

Activated states refer to continuously driven systems, or gravity free conditions. For example, a container of grains in a compact configuration can be shaken to impose kinetic energy and motion among the grains. Similarly, unrestrained systems in a gravitational field will flow towards lower potential energy (e.g., hopper flow or flow down an incline). Initial activation in space laboratory experiments provides another example (self-sustained fluidization). For the flows considered here as candidates for a hydrodynamic description continual collisions are essential. This means that within each small cell, still containing many particles, the particles are moving randomly relative to the collective motion of that cell. Thus, ballistic motion or beams with all particles moving independently in the same direction are excluded.

Both compact and activated grains may occur immersed in a continuum such as water or air that may have a strong or weak effect on their collective properties. For compact systems water may provide a lubrication effect that affects the dominant class of configurations. For activated systems it can provide an additional dissipative drag between collisions among the grains. When the medium plays an important role the systems is said to be wet. In the opposite limit it is said to be dry. Finally, it is possible for compact and activated components of a system to coexist as heterogeneous states. Here, only the simplest case of dry systems in fully activated flows are considered. These are referred to in the following as granular fluids.

Advances in the study of granular fluids have arisen from many communities, including

chemical engineering, materials sciences, and physics. The additional academic and conceptual importance of granular matter as practical systems for exploring the relevance of many-body fluid methods is primarily for the physics community. Granular matter, viewed as a system of particles with inelastic interactions, provides new opportunities to test the qualitative and quantitative limits of many-body methods developed over the past century for atomic and molecular systems. This is the field of non-equilibrium statistical mechanics [3, 4, 5]. Granular matter provides a new testing ground for a reconsideration of the most fundamental concepts and tools [1], with the potential for enhanced understanding of their place in atomic and molecular systems as well.

Statistical mechanics addresses the difficult many-body problem of extracting macroscopic properties of experimental interest from the very large number of constituent particles. The results express these properties in terms of the fundamental "microscopic" features of these particles, such as mass, shape, degree of inelasticity, and collisional properties. In this way the properties of the vitamin pills, mustard seeds, and peanuts are distinguished at a fundamental level. Also, conceptual issues such as the limitations of a macroscopic description are exposed through the insistence on their logical evolution from the fundamental microdynamics. In the next section, the granular fluid is described as a system of particles interacting via pairwise additive, nonconservative forces. The microscopic dynamics of these particles leads to balance equations for the mass density, energy density, and momentum density. Their averages define the "hydrodynamic fields" which are candidates for a macroscopic, continuum mechanics description. These exact equations are described in Section 3 and the need for "constitutive equations" to provide a closure is described. The origin of constitutive equations, and consequently the origin of hydrodynamics, is associated with the concept of "normal states" [16] in Section 4. The normal state for the case of small spatial deviations from homogeneity is constructed formally in Section 5, resulting in the constitutive equations for Navier-Stokes hydrodynamics [17]. This derivation also provides insight into the context in which such a description should hold, and differences from the corresponding results for a normal fluid are noted. Empirical evidence [18, 19], simulations [20, 21, 22], and corresponding results from kinetic theory [23, 24, 25, 26] support the applicability of this hydrodynamic description under appropriate conditions. Finally, the results are summarized in Section 6 and some comments on the outlook for future developments are offered.

The presentation here is focused on recent work of the author and his collaborators for application of statistical mechanics to explore hydrodynamics for a granular gas. Consequently, the references quoted are heavily weighted toward those developmental studies. Apologies are offered for the exclusion of the vast and important complementary literature on simulations, kinetic theory, and experiments also bearing on this topic. Many of these can be found in the list of Books and Reviews given here.

### III. GRANULAR FLUID AND ITS STATISTICAL MECHANICS

#### A. Nonequilibrium statistical mechanics

Consider a system of  $N \gg 1$  identical grains (hereafter referred to as particles) in a volume  $V$ , whose initial positions  $\{\mathbf{q}_i\}$  and velocities  $\{\mathbf{v}_i\}$ ,  $1 \leq i \leq N$ , are specified. The positions and velocities define a point in a  $6N$  dimensional space denoted by  $\Gamma \equiv \{\mathbf{q}_i, \mathbf{v}_i\}$ , defining the microstate of the system. A macrostate is defined by a probability density  $\rho(\Gamma)$  in this space, representing statistical rather than precise knowledge of the system. The field of statistical mechanics addresses properties of macrostates, based on the recognition that for very large  $N$  the details of microstates are neither experimentally accessible nor practically calculable. Properties of interest are represented by functions  $A(\Gamma)$ , and their values for a macrostate  $\rho(\Gamma)$  are determined from the expectations

$$\langle A; \rho \rangle \equiv \int d\Gamma \rho(\Gamma) A(\Gamma). \quad (3.1)$$

In this section, a brief overview of the essential ingredients of nonequilibrium statistical mechanics is given, broadened from its usual form [3] to include granular matter.

The dynamics of macrostates is determined from the underlying dynamics of the microstates. The initial point  $\Gamma$  changes in time since the particles have velocities and move to new positions. They move in straight lines until one or more come within the force field of other particles, at which point their velocities change as well as their positions. The forces are taken to be pairwise additive, such that the total force on particle  $i$  is  $\mathbf{F}_i = \sum_j \mathbf{F}_{ij}$ , where  $\mathbf{F}_{ij}$  is the force on particle  $i$  due to particle  $j$ . This does not mean that the interactions are pairwise sequential; three or more particles can interact simultaneously. The pair forces are restricted by Newton's third law,  $\mathbf{F}_{ij} = -\mathbf{F}_{ji}$ , with conservation of momentum. Otherwise quite general forces can be considered to represent the shape of the particles and their degree

of inelasticity. It is assumed here that the force range vanishes outside a distance  $\sigma/2$  from the center of each particle so that  $\sigma$  characterizes the size of the particles. Furthermore, the particles are taken to be strongly repulsive so that their mean maximum overlap  $d$  on collision is small compared to their size,  $d/\sigma < 1$ . However, their size can be large or small compared to the mean distance between particles  $(V/N)^{1/3}$ , depending on whether the density of the system is small or large, respectively. Most importantly for the purposes here, these forces do not conserve energy. This property captures the feature of real grains that center of mass kinetic energy is lost as they distort during pair collisions. Further details of the force law are not required at this point.

The dynamics consists of straight line motion along the direction of the velocity at time  $t$  (free streaming), until the force range of any pair of particles, say  $i, j$ , overlaps. The relative velocity  $\mathbf{g}_{ij} = \mathbf{v}_i - \mathbf{v}_j$  of that pair changes according to Newton's second law for the chosen force law  $\mathbf{F}_{ij}$ . Subsequently, all particles continue to stream freely until another pair has a force range of overlap, and the collisional change is repeated for that pair. In this way a trajectory  $\Gamma_t \equiv \{\mathbf{q}_1(t), \dots, \mathbf{q}_N(t), \mathbf{v}_1(t), \dots, \mathbf{v}_N(t)\}$  is generated for  $t > 0$ . This trajectory is unique and invertible. The statistical mechanics for a fluid of inelastic particles [9, 10, 11, 12] is comprised of the dynamics just described, a macrostate specified in terms of a probability density  $\rho(\Gamma)$ , and a set of observables generically denoted by  $A(\Gamma)$ . The expectation value for an observable at time  $t > 0$  for a state  $\rho(\Gamma)$  given at  $t = 0$  is defined by

$$\langle A(t); 0 \rangle \equiv \int d\Gamma \rho(\Gamma) A(\Gamma_t) \equiv \int d\Gamma \rho(\Gamma) e^{tL} A(\Gamma) \quad (3.2)$$

where  $A(t) = A(\Gamma_t)$ , and  $\Gamma_t \equiv \{\mathbf{q}_1(t), \dots, \mathbf{q}_N(t), \mathbf{v}_1(t), \dots, \mathbf{v}_N(t)\}$  is the phase point evolved to time  $t$  from  $\Gamma = \Gamma_{t=0}$ . The dynamics can be represented in terms of a generator  $L$  defined by the second equality of (3.2). There are two components to the generator, corresponding to the two steps of free streaming and velocity changes due to interactions

$$L = \sum_{i=1}^N \mathbf{v}_i \cdot \nabla_i + \frac{1}{2m} \sum_{i=1}^N \sum_{j \neq i}^N \mathbf{F}_{ij} \cdot (\nabla_{\mathbf{v}_i} - \nabla_{\mathbf{v}_j}). \quad (3.3)$$

An alternative equivalent representation of the dynamics is obtained by transferring the dynamics from the observable  $A(\Gamma)$  to the state  $\rho(\Gamma)$  by the definition

$$\int d\Gamma \rho(\Gamma) e^{tL} A(\Gamma) \equiv \int d\Gamma \left( e^{-tL} \rho(\Gamma) \right) A(\Gamma) \equiv \int d\Gamma \rho(\Gamma, t) A(\Gamma). \quad (3.4)$$

The representation in terms of a dynamical state  $\rho(\Gamma, t)$  is referred to as Liouville dynamics. Its generator  $\bar{L}$  is the formal adjoint of  $L$  which is found to be

$$\bar{L} = L + \frac{1}{2m} \sum_{i=1}^N \sum_{j \neq i}^N (\nabla_{\mathbf{v}_i} - \nabla_{\mathbf{v}_j}) \cdot \mathbf{F}_{ij} \quad (3.5)$$

The difference between  $L$  and  $\bar{L}$  arises because the forces are non-conservative and therefore depend on the relative velocities of each pair as well as their positions. Time correlation functions for two observables  $A$  and  $B$  are defined in a similar way

$$\langle A(t)B; 0 \rangle \equiv \int d\Gamma (e^{tL} A(\Gamma)) \rho(\Gamma) B(\Gamma) = \int d\Gamma A(\Gamma) (e^{-t\bar{L}} \rho(\Gamma)) (e^{-tL} B(\Gamma)). \quad (3.6)$$

or

$$\langle A(t)B; 0 \rangle \equiv \langle AB(-t); t \rangle \quad (3.7)$$

In summary, averages like  $\langle A(t); 0 \rangle$  and correlation functions  $\langle A(t)B; 0 \rangle$  are the central properties of interest for a macroscopic description of physical systems. The microscopic dynamics can be represented in terms of the observables  $A(\Gamma, t)$  or the states  $\rho(\Gamma, t)$  which are determined from specified initial values and the equations

$$(\partial_t - L) A(\Gamma, t) = 0, \quad (\partial_t + \bar{L}) \rho(\Gamma, t) = 0. \quad (3.8)$$

In the following most of the analysis is done in terms of the states, and the associated equation of motion is known as the Liouville equation.

## B. Liouville equation and cooling

For an isolated system, the total energy decreases monotonically due to the loss of energy on each pair collision. This is reflected in a decrease of the average kinetic energy of the particles between collisions and hence is referred to as collisional "cooling". The energy per particle at time  $t$  and its loss are

$$\epsilon(t) \equiv N^{-1} \langle E; t \rangle, \quad \omega(t) \equiv -\partial_t \epsilon(t) = N^{-1} \langle LE; t \rangle. \quad (3.9)$$

This cooling effect is common to all solutions to the Liouville equation and it is useful to separate the dynamics into that due to this cooling and the residual time dependence

$$\rho(\Gamma, t) \equiv \rho(\Gamma, \epsilon(t), t). \quad (3.10)$$

The Liouville equation then can be written

$$\partial_t \rho(\Gamma, \epsilon, t) |_\epsilon + (-\omega(\epsilon, t) \partial_\epsilon + \bar{L}) \rho(\Gamma, \epsilon, t) = 0. \quad (3.11)$$

The time derivative is now taken at constant  $\epsilon$ . The notation  $\omega(\epsilon, t)$  reflects the fact that it is a linear functional of  $\rho(\Gamma, \epsilon, t)$ , from its definition (3.9). This is a useful form that isolates a primary effect of the nonconservative forces (cooling) from the residual dynamics that will be associated with relaxation of the spatial inhomogeneities of interest below. For notational simplicity (3.11) is written

$$(\partial_t + \bar{\mathcal{L}}) \rho(\Gamma, \epsilon, t) = 0, \quad \bar{\mathcal{L}} \equiv -\omega(\epsilon, t) \partial_\epsilon + \bar{L}. \quad (3.12)$$

The corresponding equation for observables is

$$(\partial_t - \mathcal{L}) A(\Gamma, \epsilon, t) = 0, \quad \mathcal{L} \equiv -\partial_\epsilon \omega(\epsilon, t) + L. \quad (3.13)$$

where it is understood that  $\partial_\epsilon$  operates on everything to its right.

### C. Stationary homogeneous state

An isolated normal fluid supports an equilibrium state. This is a stationary solution to the Liouville equation with translational invariance, the Gibbs states. From the discussion above it is clear that isolated granular fluids have no truly stationary state due to cooling. However, there is a "universal" homogeneous state similar to the Gibbs state in the sense that a wide class of homogeneous initial states rapidly approach this state, on the time scale of a few collisions per particle. It is simple in the sense that all of its time dependence is that associated with cooling

$$\rho_0(\Gamma, t) = \rho_0(\{\mathbf{q}_{ij}, \mathbf{v}_i\}, \epsilon(t)). \quad (3.14)$$

Here,  $\mathbf{q}_{ij} = \mathbf{q}_i - \mathbf{q}_j$  so the solution also has translational invariance. In the representation (3.12) it is seen to be a stationary solution to the Liouville equation

$$\bar{\mathcal{L}} \rho_0 = 0. \quad (3.15)$$

There is no longer any explicit time dependence since  $\omega(\epsilon, t) = \omega(\epsilon)$  and  $\bar{\mathcal{L}} = -\omega(\epsilon) \partial_\epsilon + \bar{L}$  for this state. This solution is referred to as the homogeneous cooling state (HCS). Clearly, it is the close analogue of the Gibbs state for a normal fluid. It is an example of a "normal" state in the sense that all of its time dependence occurs through one of the hydrodynamic fields (the energy). This concept is sharpened below.



#### IV. MACROSCOPIC BALANCE EQUATIONS

The origins of a macroscopic description for a fluid are the balance equations for the average mass density  $\langle m(\mathbf{r}); t \rangle$ , energy density  $\langle e(\mathbf{r}); t \rangle$ , and momentum density  $\langle \mathbf{g}(\mathbf{r}); t \rangle$ , where  $\mathbf{r}$  denotes an arbitrary field point within the system [16]. These will be referred to as the hydrodynamic fields since they are the ones that are expected to obey the hydrodynamic equations under appropriate conditions. The phase functions  $m(\Gamma, \mathbf{r})$ ,  $e(\Gamma, \mathbf{r})$ , and  $\mathbf{g}(\Gamma, \mathbf{r})$  are well known and their explicit forms will not be needed here. They will be denoted collectively by  $a_\alpha(\mathbf{r})$

$$a_\alpha(\mathbf{r}, t) \leftrightarrow \{m(\mathbf{r}), e(\mathbf{r}), \mathbf{g}(\mathbf{r})\}. \quad (4.1)$$

It follows from (3.8) that they obey the microscopic balance equations [14]

$$\partial_t a_\alpha(\mathbf{r}, t) = L a_\alpha(\mathbf{r}, t) = -\nabla \cdot \mathbf{b}_\alpha(\mathbf{r}, t) - \delta_{\alpha 2} w(\mathbf{r}, t). \quad (4.2)$$

To obtain this result, it has been recognized that the quantity  $L a_\alpha(\mathbf{r}, t)$  can be written as the sum of a divergence  $\nabla \cdot \mathbf{b}_\alpha(\mathbf{r}, t)$  plus a remainder  $w(\mathbf{r}, t)$  that cannot be so represented. For a normal fluid  $w(\mathbf{r}, t)$  vanishes and (4.2) become the local conservation laws for mass, energy, and momentum. The  $\mathbf{b}_\alpha(\mathbf{r}, t)$  are the corresponding fluxes. This clarifies why  $a_\alpha(\mathbf{r}, t)$  are selected for a macroscopic description. Their time dependence is determined by the scale of the spatial gradients of the fluxes, and averages of the latter become small as the system approaches homogeneity. Consequently, on long time scales the  $\langle a_\alpha(\mathbf{r}); t \rangle$  are the only surviving dynamical variables, and it is under these conditions that these fields obey hydrodynamic equations. The mass and momentum are conserved for a granular fluid as well, but there is a loss of energy  $w(\mathbf{r}, t)$  due to the non-conservative forces. It is no longer obvious that the energy is still one of the slow variables since its time scale is coupled to  $w(\mathbf{r}, t)$  which does not become small for nearly homogeneous states. Thus, an additional requirement for the existence of a macroscopic description in terms of  $\langle a_\alpha(\mathbf{r}); t \rangle$  is that the time scale of  $\langle e(\mathbf{r}); t \rangle / \langle w(\mathbf{r}); t \rangle$  must be larger than that for non-hydrodynamic properties. This issue is discussed further below.

The macroscopic balance equations follow from the averages of (4.2)

$$\partial_t \langle a_\alpha(\mathbf{r}); t \rangle + \nabla \cdot \langle \mathbf{b}_\alpha(\mathbf{r}); t \rangle = -\delta_{\alpha 2} \langle w(\mathbf{r}); t \rangle. \quad (4.3)$$

These equations are formally exact, but of little practical use as they do not form a closed (self-deterministic) set of equations for  $\langle a_\alpha(\mathbf{r}); t \rangle$ . Closure requires expressing the aver-

age flux  $\langle \mathbf{b}_\alpha(\mathbf{r}); t \rangle$  and energy loss  $\langle w(\mathbf{r}); t \rangle$  as functionals of the fields  $\langle a_\alpha(\mathbf{r}); t \rangle$ . Such relationships are called "constitutive equations". The combination of the exact balance equations with some form of constitutive equations provides the most general definition of hydrodynamics.

Construction of the constitutive equations is simplified by extracting the effects of convection. The velocity  $\mathbf{U}(\mathbf{r}, t)$  of a cell at point  $\mathbf{r}$  is defined in terms of the average momentum

$$\langle \mathbf{g}(\mathbf{r}); t \rangle \equiv \langle m(\mathbf{r}); t \rangle \mathbf{U}(\mathbf{r}, t). \quad (4.4)$$

The fluxes are functions of the positions and velocities  $\mathbf{b}_\alpha(\mathbf{r}) = \mathbf{b}_\alpha(\mathbf{r}; \{\mathbf{q}_i, \mathbf{v}_i\}) = \mathbf{b}_\alpha(\mathbf{r}; \{\mathbf{q}_i, \mathbf{V}_i + \mathbf{U}(\mathbf{r})\})$ , where the velocity in the local rest frame has been introduced,  $\mathbf{V}_i = \mathbf{v}_i - \mathbf{U}(\mathbf{r}, t)$ . Then defining the microscopic flux in the rest frame by  $\mathbf{b}'_\alpha(\mathbf{r}) = \mathbf{b}_\alpha(\mathbf{r}; \{\mathbf{q}_i, \mathbf{V}_i\})$  it follows that the average flux has the form [3]

$$\langle \mathbf{b}_\alpha(\mathbf{r}); t \rangle = \langle \mathbf{b}'_\alpha(\mathbf{r}); t \rangle + \mathbf{c}_{\alpha\eta} \mathbf{U}(\mathbf{r}, t) \cdot \langle \mathbf{b}'_\eta(\mathbf{r}); t \rangle + \mathbf{U}(\mathbf{r}, t) d_\alpha(\{\langle a_\nu(\mathbf{r}); t \rangle\}). \quad (4.5)$$

The first term is the flux of mass, energy, and momentum in a fluid element at rest, and represents the dissipative processes. The second and third terms are proportional to the flow velocity  $\mathbf{U}(\mathbf{r}, t)$  and are associated with convection. The coefficients of these terms are explicit functions of the fields  $\langle a_\alpha(\mathbf{r}); t \rangle$  (as is  $\mathbf{U}(\mathbf{r}, t)$ ). For a normal fluid, neglect of the rest frame fluxes leads to the perfect fluid Euler hydrodynamic equations. Hence, determination of the constitutive equations is reduced to expressing the rest frame fluxes and energy loss as functionals of the fields.

## V. "NORMAL" STATES AND HYDRODYNAMICS

A hydrodynamic description is a closed set of equations for the hydrodynamic fields,  $\langle a_\alpha(\mathbf{r}); t \rangle$ . This follows from the exact macroscopic balance equations if the energy loss and fluxes can be represented as functionals of these fields

$$\langle w(\mathbf{r}); t \rangle \rightarrow \omega(\mathbf{r} \mid \langle a_\alpha; t \rangle), \quad \langle \mathbf{b}_\alpha(\mathbf{r}); t \rangle \rightarrow \beta_\alpha(\mathbf{r} \mid \langle a_\alpha; t \rangle). \quad (5.1)$$

The arrow is used to indicate that such a functional representation need not be valid on all length and time scales, and any such restrictions constitute the domain of validity for hydrodynamics. The notation here and below is such that  $f(\mathbf{r}, t, \{\langle a_\alpha(\mathbf{r}); t \rangle\})$  denotes a

*function* of  $\mathbf{r}, t$  and of the fields  $\langle a_\alpha(\mathbf{r}); t \rangle$  at the point  $\mathbf{r}$ , while  $f(\mathbf{r}, t | \langle a_\alpha; t \rangle)$  denotes a function of  $\mathbf{r}, t$  and a *functional* of the  $\langle a_\alpha; t \rangle$  at all space points. With such constitutive relations the macroscopic balance equations (4.3) become hydrodynamic equations

$$\partial_t \langle a_\alpha(\mathbf{r}); t \rangle + \nabla \cdot \beta(\mathbf{r} | \langle a_\alpha; t \rangle) = -\delta_{\alpha 2} \omega(\mathbf{r} | \langle a_\alpha; t \rangle). \quad (5.2)$$

The average energy loss and fluxes are averages of specific functions of the particle positions and velocities, and hence are linear functionals of the solution to the Liouville equation. The existence of constitutive equations is therefore related to a special property of the solution which will be called "normal" (this terminology originates in a related context for derivation of hydrodynamics from the Boltzmann kinetic equation [3]). The class of "normal" distributions is defined by the functional forms

$$\rho_n(\Gamma, t) = \rho_n(\{\mathbf{q}_{ij}, \mathbf{v}_i\} | \langle a_\alpha; t \rangle). \quad (5.3)$$

All time dependence and all the breaking of translational invariance for normal states occurs only through the hydrodynamic fields. A familiar example of a normal distribution for real fluids is the *local* Gibbs distribution

$$\rho_{el}(\Gamma | \langle a_\alpha; t \rangle) = \exp \left\{ q - \int d\mathbf{r} y_\alpha(\mathbf{r}, t) a_\alpha(\mathbf{r}) \right\} \quad (5.4)$$

Here  $q$  is a normalization constant, and  $y_\alpha(\mathbf{r}, t)$  are conjugate fields determined by the requirement that the averages of  $a_\alpha(\mathbf{r})$  give the specified values  $\langle a_\alpha(\mathbf{r}); t \rangle$ . In this way  $y_\alpha(\mathbf{r}, t)$  are functionals of the hydrodynamic fields and  $\rho_{el}(\Gamma | \langle a_\alpha; t \rangle)$  is normal. The importance of normal solutions is that they yield directly the desired functionals of (5.1)

$$\omega(\mathbf{r} | \langle a_\alpha; t \rangle) = \int d\Gamma \rho_n(\Gamma | \langle a_\alpha; t \rangle) w(\mathbf{r}) \quad (5.5)$$

$$\beta_\alpha(\mathbf{r} | \langle a_\alpha; t \rangle) = \int d\Gamma \rho_n(\Gamma | \langle a_\alpha; t \rangle) \mathbf{b}_\alpha(\mathbf{r}) \quad (5.6)$$

The normal state in (5.5) and (5.6) must be a solution to the Liouville equation. In general, the time derivative in the Liouville equation can be separated into that which occurs through  $\langle a_\alpha; t \rangle$  plus the residual time dependence, generalizing (3.10)

$$\rho(\Gamma, t) = \rho(\Gamma, t | \langle a_\alpha; t \rangle). \quad (5.7)$$

The Liouville equation then becomes

$$\partial_t \rho |_{\langle a_\alpha; t \rangle} - \int d\mathbf{r} \frac{\delta \rho}{\delta \langle a_\alpha(\mathbf{r}); t \rangle} \{ \nabla \cdot \langle \mathbf{b}_\alpha(\mathbf{r}); t \rangle + \delta_{\alpha 2} \langle w(\mathbf{r}); t \rangle \} + \bar{L} \rho = 0. \quad (5.8)$$

A normal solution results when  $\partial_t \rho_n |_{\langle a_\alpha; t \rangle} \rightarrow 0$ . For specified fields, (5.8) becomes an equation for the  $\Gamma$  dependence of the normal phase space density as a functional of the fields. This dependence then allows determination of the normal forms in (5.5) and (5.6). Finally, with the form of the hydrodynamic equation determined at that point, their solution with suitable initial and boundary conditions provides the explicit forms for the fields, and completes the normal solution. The existence and determination of this solution is the central problem for establishing a hydrodynamic description for both normal and granular fluids.

The concept of a normal solution and its use in the macroscopic balance equations makes no special reference to whether the fluid is normal or granular, and is not restricted to states near homogeneity. In this general context, hydrodynamics is not a simple set of local partial differential equations such as the familiar Navier-Stokes equations. The latter are a special case of this more general idea, and their inadequacy for some conditions should not be interpreted as the absence of a more complex hydrodynamic description.

In closing this Section a qualitative explanation of why a normal solution can be expected is given, by analogy with the similar expectation for atomic fluids. For a wide class of initial states there is a first stage of rapid velocity relaxation in each small region toward the universal homogeneous state (HCS or Gibbs, respectively). However, the hydrodynamic parameters of that universal state are specific to each region so it is only locally homogeneous, as in (5.4) for the atomic fluid. Subsequently, these differences in the parameters of neighboring cells are decreased by the fluxes of mass, energy, and momentum across their boundaries. It is this second stage where a normal description in terms of the hydrodynamic fields can be expected, indicating also that the space and time scales for a hydrodynamic description should be large compared to those of the first stage. This basic conceptual picture is essentially the same for both atomic and granular fluids, and the rapid approach of the first stage is indeed observed in molecular dynamics simulation studies of both equilibrium and the HCS.

## VI. NAVIER-STOKES APPROXIMATION

Equation (5.8) presents a formidable problem and further progress requires specialization to specific cases of interest. Perhaps the simplest of these are weakly inhomogeneous states. These are states for which all spatial gradients of first order are small and all higher order

derivatives are negligible. Small gradients means that the relative change in the hydrodynamic fields over the largest microscopic length scale  $\ell_0$  is small:  $\ell_0 \partial_r \ln \langle a_\alpha; t \rangle \ll 1$ . There are two characteristic length scales, the mean free path and the grain diameter. For a dilute gas the mean free path is largest, while for a dense fluid the grain size is largest. Under these conditions a solution to the Liouville equation can be sought as an expansion to leading order in these small gradients. This will be referred to as the Navier-Stokes approximation.

According to the discussion at the end of the last section, a normal solution is expected after the system has relaxed to its local HCS form, denoted by  $\rho_{0\ell}(\Gamma \mid \langle a_\alpha; t \rangle)$ , representing the fluid as having each cell in its own HCS. Define the deviations of the hydrodynamic fields from some common reference value by

$$\delta \langle a_\alpha; t \rangle = \langle a_\alpha; t \rangle - a_{0\alpha}, \quad (6.1)$$

where  $a_{0\alpha}$  is the same for all cells. Then, the local HCS must satisfy the conditions

$$\rho_{0\ell}(\Gamma \mid a_{0\alpha} + \delta \langle a_\alpha; t \rangle) \big|_{\delta \langle a_\alpha; t \rangle = 0} = \rho_0(\Gamma; a_{0\alpha}), \quad (6.2)$$

$$\frac{\partial \rho_0}{\partial a_{0\alpha}} = \int d\mathbf{r} \frac{\delta \rho_{0\ell}(\Gamma \mid a_{0\alpha} + \delta \langle a_\alpha; t \rangle)}{\delta \langle a_\alpha(\mathbf{r}); t \rangle_\alpha} \big|_{\delta \langle a_\alpha; t \rangle = 0}, \dots \quad (6.3)$$

i.e., the local HCS and all of its functional derivatives must agree with those of the HCS in the homogenous limit. Also, as a normal distribution its time dependence is through the exact hydrodynamic fields for the fluid state considered. This means the averages of the corresponding microscopic fields  $a_\alpha(\mathbf{r})$  for the local HCS and for the solution to the Liouville equation must be the same

$$\int d\Gamma (\rho - \rho_{0\ell}) a_\alpha(\mathbf{r}) = 0. \quad (6.4)$$

A more complete discussion of the construction of  $\rho_{0\ell}$  from knowledge of  $\rho_0$  is given elsewhere [14]. For the purposes here properties (6.2), (6.3), and (6.4) are sufficient.

The local HCS distribution,  $\rho_{0\ell}$ , is not a solution to the Liouville equation except in limit that all hydrodynamic fields become the same for each cell. Instead, it is a reference state approximating the actual solution after its first stage of velocity relaxation. To construct a solution  $\rho$  define its deviation from  $\rho_{0\ell}$  by

$$\rho(\Gamma, t \mid \langle a_\alpha; t \rangle) = \rho_{0\ell}(\Gamma, t \mid \langle a_\alpha; t \rangle) + \Delta(\Gamma, t \mid \langle a_\alpha; t \rangle). \quad (6.5)$$

The Liouville equation (5.8) gives

$$\begin{aligned} & \partial_t \Delta - \int d\mathbf{r}' \frac{\delta \Delta}{\delta \langle a_\alpha(\mathbf{r}') ; t \rangle} \{ \nabla \cdot \langle \mathbf{b}_\alpha(\mathbf{r}) ; t \rangle + \delta_{\alpha 2} \langle w(\mathbf{r}) ; t \rangle \} + \bar{L} \Delta \\ &= \int d\mathbf{r}' \frac{\delta \rho_{0\ell}}{\delta \langle a_\alpha(\mathbf{r}') ; t \rangle} \{ \nabla \cdot \langle \mathbf{b}_\alpha(\mathbf{r}) ; t \rangle + \delta_{\alpha 2} \langle w(\mathbf{r}) ; t \rangle \} - \bar{L} \rho_{0\ell}. \end{aligned} \quad (6.6)$$

This equation is still exact, but if only small gradient states are considered it simplifies by retaining terms only of first order in the gradients. To be precise, the ultimate use of this solution is to calculate local properties of the form

$$A(\mathbf{r}, t | \{y_\alpha(t)\}) = \int d\Gamma a(\Gamma, \mathbf{r}) \rho(\Gamma, t | \langle a_\alpha(\mathbf{r}) ; t \rangle + \delta \langle a_\alpha ; t \rangle). \quad (6.7)$$

Therefore, in the following analysis the gradient expansions are referred to the field point  $\mathbf{r}$  of interest,  $\langle a_\alpha ; t \rangle = \langle a_\alpha(\mathbf{r}) ; t \rangle + \delta \langle a_\alpha ; t \rangle$ , i.e. the common reference values in (6.1) are the exact field values at the chosen point,  $a_{0\alpha} = \langle a_\alpha(\mathbf{r}) ; t \rangle$ . The gradient expansion is carried out relative to these values. Of course the results will be general and applicable to any choice for  $\mathbf{r}$ .

The details of the gradient expansion are given in the Appendix. The solution to the Liouville equation to first order in the gradients is

$$\begin{aligned} \rho(\Gamma, t | \langle a_\alpha ; t \rangle) &= \rho_0(\Gamma, \langle a_\alpha(\mathbf{r}) ; t \rangle) + (1 - \mathcal{P})(\mathbf{M}_\beta(\Gamma, \langle a_\alpha(\mathbf{r}) ; t \rangle) \\ &+ \int_0^t dt' \left( e^{-(I\bar{\mathcal{L}} + K^T)t'} \right)_{\beta\nu} (1 - \mathcal{P}) \Upsilon_\nu(\Gamma, \langle a_\alpha(\mathbf{r}) ; t \rangle) \cdot \nabla \langle a_\beta(\mathbf{r}) ; t \rangle. \end{aligned} \quad (6.8)$$

with the definitions

$$\mathbf{M}_\beta = \int d\mathbf{r}' \left( \frac{\delta \rho_{0\ell}}{\delta \langle a_\alpha(\mathbf{r}') ; t \rangle} \right)_{\delta \langle a_\alpha ; t \rangle = 0} \mathbf{r}', \quad (6.9)$$

$$\Upsilon_\alpha = -(I\bar{\mathcal{L}} + K^T)_{\alpha\beta} \mathbf{M}_\beta. \quad (6.10)$$

The generator for the dynamics  $I\bar{\mathcal{L}} + K^T$  has a contribution from  $\bar{\mathcal{L}}$  which is the same as in (3.12), with  $\omega$  evaluated for the HCS as a function of the exact hydrodynamic fields at the point  $\mathbf{r}$  and time  $t$

$$\bar{\mathcal{L}} = -\omega_0(\langle a_\alpha(\mathbf{r}) ; t \rangle) \partial_{\langle e(\mathbf{r}) ; t \rangle} + \bar{L}. \quad (6.11)$$

The second contribution to the generator of the dynamics is the transpose of the matrix  $K_{\alpha\beta}$

$$K_{\alpha\beta} = \delta_{\alpha 2} \frac{\partial \omega_0(\langle a_\alpha(\mathbf{r}) ; t \rangle)}{\partial \langle a_\beta(\mathbf{r}) ; t \rangle}. \quad (6.12)$$

Finally,  $\mathcal{P}$  is a projection operator

$$\mathcal{P}X = \Psi_\beta \int d\Gamma A_\beta X, \quad A_\beta = V^{-1} \int d\mathbf{r} a_\beta(\mathbf{r}), \quad \Psi_\beta \equiv \frac{\partial \rho_0}{\partial \langle a_\beta(\mathbf{r}); t \rangle} \quad (6.13)$$

The phase functions  $A_\beta$  and  $\Psi_\beta$  form a biorthogonal set in the sense

$$\int d\Gamma A_\alpha \Psi_\beta = \delta_{\alpha\beta}. \quad (6.14)$$

The  $A_\alpha$  are the usual global invariants of the Liouville operator  $\bar{L}$  for a normal fluid; it is shown in the Appendix that the  $\Psi_\beta$  are the invariants of the new generator for dynamics in a granular fluid

$$(I\bar{\mathcal{L}}_T + K^T)_{\nu\beta} \Psi_\beta = 0. \quad (6.15)$$

Equation (6.8) is not quite the normal solution desired. All terms depend on time through  $\langle a_\beta(\mathbf{r}); t \rangle$  as required, except for the last term which has an additional explicit time dependence through the upper limit of the time integral. This time dependence becomes negligible if the integrand is effectively non-zero after some short time scale  $\tau$ . Then for  $t \gg \tau$  the time integral becomes independent of  $t$  and can be taken formally to infinity. Thus, a normal solution is attained for this time scale

$$\begin{aligned} \rho_n(\Gamma, \langle a_\alpha(\mathbf{r}); t \rangle) &= \rho_0(\Gamma, \langle a_\alpha(\mathbf{r}); t \rangle) + (1 - \mathcal{P})(\mathbf{M}_\beta(\Gamma, \langle a_\alpha(\mathbf{r}); t \rangle)) \\ &\quad + \lim_{t_0 \rightarrow \infty} \int_0^{t_0} dt' \left( e^{-(I\bar{\mathcal{L}} + K^T)t'} \right)_{\beta\nu} (1 - \mathcal{P}) \Upsilon_\nu(\Gamma, \langle a_\alpha(\mathbf{r}); t \rangle) \cdot \nabla \langle a_\beta(\mathbf{r}); t \rangle. \end{aligned} \quad (6.16)$$

It is expected that the integrand should have this property of a short time scale since the domain of operation for the generator of time dependence is functions with translational invariance (as a consequence of the gradient expansion). Hence there are no explicit slow hydrodynamic modes of finite wavelength. Also, there is no contribution from the homogeneous hydrodynamics (that for the invariants) due to the orthogonal projection  $(1 - \mathcal{P})$ . The appearance of this projection is an essential self-consistency of the analysis, and occurs as well for normal fluids. The expression (6.16) is only formal and the actual limit should be taken in the weak sense only after (6.8) has been used to define average properties. A technical complication is the occurrence of periodic time dependence, the Poincare recurrence time. This can be removed by considering the thermodynamic limit of  $V \rightarrow \infty, N \rightarrow \infty$  at constant  $N/V$ . Therefore, averages using the normal solution to the Liouville equation are

understood as having the thermodynamic limit followed by the long time limit at constant  $\langle a_\alpha(\mathbf{r}); t \rangle$ .

An alternative equivalent form results from performing the integral in (6.16) using the explicit form (6.10) and the property (22) of the Appendix

$$\begin{aligned} \rho_n(\Gamma, \langle a_\alpha(\mathbf{r}); t \rangle) &= \rho_0(\Gamma, \langle a_\alpha(\mathbf{r}); t \rangle) \\ &+ \lim_{t_0 \rightarrow \infty} (1 - \mathcal{P}) \left( e^{-(I\bar{\mathcal{L}} + K^T)t_0} \right)_{\beta\nu} \mathbf{M}_\nu(\Gamma, \langle a_\alpha(\mathbf{r}); t \rangle) \cdot \nabla \langle a_\beta(\mathbf{r}); t \rangle. \end{aligned} \quad (6.17)$$

The decay time for the integrand of (6.16) now becomes the time after which (6.17) reaches its normal form.

### A. Constitutive equations

The exact macroscopic balance equations are given by (5.2), and the necessary constitutive equations are given by (5.5) and (5.6) as averages over the normal solution. These can be made more explicit now using the small gradient result (6.16). Since the latter is a local function of the fields, the constitutive equations also will be local. Furthermore, since all components of the gradients in (6.17) depend on the common value  $\langle \mathbf{g}(\mathbf{r}); t \rangle$ , this can be eliminated through a Galilean transformation so that all properties refer to a fluid element at rest. Of course, the gradients of  $\langle \mathbf{g}(\mathbf{r}); t \rangle$  in that fluid element are nonzero.

Consider first the energy loss function  $\omega$

$$\omega(\langle a_\alpha(\mathbf{r}); t \rangle) = \int d\Gamma \rho_n(\Gamma, \langle a_\alpha(\mathbf{r}); t \rangle) w(\mathbf{r}) = \int d\Gamma \rho_n(\Gamma, \langle a_\alpha(\mathbf{r}); t \rangle) \bar{w}. \quad (6.18)$$

The coefficients of the gradient in the normal solution have translational invariance and the average is independent of  $\mathbf{r}$ , except through its parameterization by  $\langle a_\alpha(\mathbf{r}); t \rangle$ . The second equality takes this into account by replacing  $w(\mathbf{r})$  by its average  $\bar{w}$

$$\bar{w} = V^{-1} \int d\mathbf{r} w(\mathbf{r}). \quad (6.19)$$

Since  $\omega(\langle a_\alpha(\mathbf{r}); t \rangle)$  is a scalar, fluid symmetry restricts the contributions to first order in the gradients to

$$\omega(\langle a_\alpha(\mathbf{r}); t \rangle) = \omega_0(\langle a_\alpha(\mathbf{r}); t \rangle) + \omega_1(\langle a_\alpha(\mathbf{r}); t \rangle) \nabla \cdot \mathbf{U}(\mathbf{r}, t). \quad (6.20)$$



Here, the flow velocity  $\mathbf{U}(\mathbf{r}, t)$  of (4.4) has been used in place of the momentum density. The first term is the contribution from the HCS distribution

$$\omega_0(\langle a_\alpha(\mathbf{r}); t \rangle) = \int d\Gamma \rho_0(\Gamma, \langle a_\alpha(\mathbf{r}); t \rangle) \bar{w}. \quad (6.21)$$

The coefficient of  $\nabla \cdot \mathbf{U}(\mathbf{r}, t)$  is

$$\omega_1(\langle a_\alpha(\mathbf{r}); t \rangle) = \lim_{t_0 \rightarrow \infty} C_\omega(t_0, \langle a_\alpha(\mathbf{r}); t \rangle) = C_\omega(0, \langle a_\alpha(\mathbf{r}); t \rangle) + \lim_{t_0 \rightarrow \infty} \int_0^{t_0} \partial_{t'} C_\omega(t', \langle a_\alpha(\mathbf{r}); t \rangle) dt' \quad (6.22)$$

with the correlation function defined by

$$C_\omega(t) = \int d\Gamma \bar{w} (1 - \mathcal{P}) e^{-\bar{\mathcal{L}}t} M_U, \quad (6.23)$$

$$M_U \equiv \frac{1}{3} \int d\mathbf{r}' \mathbf{r}' \cdot \left( \frac{\delta \rho_{0\ell}}{\delta \mathbf{U}(\mathbf{r}', t)} \right)_{\delta \langle a_\alpha; t \rangle = 0}. \quad (6.24)$$

The coefficient  $\omega_0$  defines an "equation of state" for the granular hydrodynamics, and gives the first non-trivial result of this analysis. It is similar to the pressure (given below) and is an inherent property of the local state of each cell, independent of the gradients between cells. In contrast,  $\omega_1$  is a true transport coefficient characterizing communication between cells. The first equality of (6.22) provides the Helfand form for this coefficient, while the second equality gives the equivalent Green-Kubo form. Each has its practical utility, depending on the method used for its approximate evaluation. Both forms have proven useful for normal fluids, and further discussion is provided below. Both  $\omega_0$  and the transport coefficient  $\omega_1$  vanish for normal fluids since they characterize collisional energy loss.

The fluxes  $\beta_\alpha$  of (5.6) can be determined in a similar way. As indicated in (4.5), only the rest frame flux  $\beta'_\alpha$  is required. Furthermore, since all components of the gradients in (6.17) depend on the common value  $\langle \mathbf{g}(\mathbf{r}); t \rangle$ , this can be eliminated through a Galilean transformation so that all properties refer to a fluid element at rest. Of course, the gradients of  $\langle \mathbf{g}(\mathbf{r}); t \rangle$  in that fluid element are nonzero. The component  $\beta'_1$  is the rest frame mass flux which is expected to vanish in order to give the continuity equation. This follows from the fact that  $\mathbf{b}'_1(\mathbf{r})$  is the microscopic momentum density

$$\beta'_1 = \int d\Gamma \mathbf{g}(\mathbf{r}) \rho_0(\Gamma, \langle a_\alpha(\mathbf{r}); t \rangle) + \lim_{t_0 \rightarrow \infty} \int d\Gamma \mathbf{g}(\mathbf{r}) (1 - \mathcal{P}) (\dots) = 0 \quad (6.25)$$

The first term vanishes since  $\langle \mathbf{g}(\mathbf{r}); t \rangle = 0$  in the rest frame, and the second term vanishes since  $(1 - \mathcal{P})$  projects orthogonal to the mass, energy, and momentum. Thus, the expected continuity equation is verified.

The fluxes  $\beta'_2$  and  $\beta'_\alpha$  for  $\alpha = 3, 4, 5$  are the rest frame energy and momentum fluxes. The energy flux transforms like a vector and therefore fluid symmetry (translational and rotational invariance) requires that it can depend only on gradients of scalars

$$\beta'_2 = -\lambda(\langle a_\alpha(\mathbf{r}); t \rangle) \nabla T(\mathbf{r}, t) - \mu(\langle a_\alpha(\mathbf{r}); t \rangle) \nabla \langle m(\mathbf{r}); t \rangle. \quad (6.26)$$

To make the connection with Fourier's law for an atomic fluid, a temperature  $T(\mathbf{r}, t)$  has been introduced through the definition

$$\langle e(\mathbf{r}); t \rangle \equiv e_0(\langle m(\mathbf{r}); t \rangle, T(\mathbf{r}, t)). \quad (6.27)$$

For an atomic fluid the function  $e_0(\langle m(\mathbf{r}); t \rangle, T(\mathbf{r}, t))$  is chosen to be the thermodynamic internal energy density. As there is no thermodynamics for a granular fluid this function is arbitrary and simply constitutes a change of variables from  $\langle e(\mathbf{r}); t \rangle, \langle m(\mathbf{r}); t \rangle$  to  $T(\mathbf{r}, t), \langle m(\mathbf{r}); t \rangle$ . In this form (6.26) is a generalization of Fourier's law where  $\lambda$  is the thermal conductivity [27]. The contribution from the gradient of the mass density is new to granular fluids ( $\mu = 0$  for atomic fluids). These coefficients are given by

$$\lambda(\langle a_\alpha(\mathbf{r}); t \rangle) = \lim_{t_0 \rightarrow \infty} C_\lambda(t_0, \langle a_\alpha(\mathbf{r}); t \rangle) = C_\lambda(0, \langle a_\alpha(\mathbf{r}); t \rangle) + \lim_{t_0 \rightarrow \infty} \int_0^{t_0} \partial_{t'} C_\lambda(t', \langle a_\alpha(\mathbf{r}); t \rangle) dt' \quad (6.28)$$

$$\mu(\langle a_\alpha(\mathbf{r}); t \rangle) = \lim_{t_0 \rightarrow \infty} C_\mu(t_0, \langle a_\alpha(\mathbf{r}); t \rangle) = C_\mu(0, \langle a_\alpha(\mathbf{r}); t \rangle) + \lim_{t_0 \rightarrow \infty} \int_0^{t_0} \partial_{t'} C_\mu(t', \langle a_\alpha(\mathbf{r}); t \rangle) dt' \quad (6.29)$$

with the correlation functions

$$C_\lambda(t) = \frac{1}{3} \int d\Gamma \beta'_2 \cdot (1 - \mathcal{P}) e^{-(\bar{\mathcal{L}} + K_{22})t} \mathbf{M}_T, \quad (6.30)$$

$$\begin{aligned} C_\mu(t) = & \frac{1}{3} \int d\Gamma \beta'_2 \cdot (1 - \mathcal{P}) \left( e^{-\bar{\mathcal{L}}t} \left( \mathbf{M}_m + \frac{K_{21}}{K_{22}} \mathbf{M}_T \right) \right. \\ & \left. + e^{-(\bar{\mathcal{L}} + K_{22})t} \left( \frac{\partial e_0}{\partial \langle m(\mathbf{r}); t \rangle} - \frac{K_{21}}{K_{22}} \right) \frac{\partial T}{\partial e_0} \Big|_{\langle m(\mathbf{r}); t \rangle} \mathbf{M}_T \right), \end{aligned} \quad (6.31)$$

$$\mathbf{M}_T \equiv \int d\mathbf{r}' \mathbf{r}' \left( \frac{\delta \rho_{0\ell}}{\delta T(\mathbf{r}', t)} \right)_{\delta \langle a_\alpha; t \rangle = 0}. \quad (6.32)$$

$$\mathbf{M}_m \equiv \int d\mathbf{r}' \mathbf{r}' \left( \frac{\delta \rho_{0\ell}}{\delta \langle m(\mathbf{r}') ; t \rangle} \right)_{\delta \langle a_\alpha ; t \rangle = 0}. \quad (6.33)$$

Finally, the set of vectors  $\beta'_\alpha$  for  $\alpha = 3, 4, 5$  define the pressure tensor  $\beta'_\alpha \Leftrightarrow P_{ij}$ . Fluid symmetry then determines that it can couple only to the momentum gradients, or equivalently the flow velocity gradients, in the form

$$P_{ij} = p(\langle a_\alpha(\mathbf{r}) ; t \rangle) \delta_{ij} - \eta(\langle a_\alpha(\mathbf{r}) ; t \rangle) \left( \partial_i U_j(\mathbf{r}, t) + \partial_j U_i(\mathbf{r}, t) - \frac{2}{3} \delta_{ij} \nabla \cdot \mathbf{U}(\mathbf{r}, t) \right) - \kappa(\langle a_\alpha(\mathbf{r}) ; t \rangle) \delta_{ij} \nabla \cdot \mathbf{U}(\mathbf{r}, t). \quad (6.34)$$

The scalar function  $p(\langle a_\alpha(\mathbf{r}) ; t \rangle)$  is the pressure, now identified as

$$p(\langle a_\alpha(\mathbf{r}) ; t \rangle) = \int d\Gamma \rho_0(\Gamma, \langle a_\alpha(\mathbf{r}) ; t \rangle) \beta'_{3x}. \quad (6.35)$$

The transport coefficients in (6.34) are the shear viscosity  $\eta(\langle a_\alpha(\mathbf{r}) ; t \rangle)$  and the bulk viscosity  $\kappa(\langle a_\alpha(\mathbf{r}) ; t \rangle)$  given by

$$\eta(\langle a_\alpha(\mathbf{r}) ; t \rangle) = \lim_{t_0 \rightarrow \infty} C_\eta(t_0, \langle a_\alpha(\mathbf{r}) ; t \rangle) = C_\eta(0, \langle a_\alpha(\mathbf{r}) ; t \rangle) + \lim_{t_0 \rightarrow \infty} \int_0^{t_0} \partial_{t'} C_\eta(t', \langle a_\alpha(\mathbf{r}) ; t \rangle) dt' \quad (6.36)$$

$$\kappa(\langle a_\alpha(\mathbf{r}) ; t \rangle) = \lim_{t_0 \rightarrow \infty} C_\kappa(t_0, \langle a_\alpha(\mathbf{r}) ; t \rangle) = C_\kappa(0, \langle a_\alpha(\mathbf{r}) ; t \rangle) + \lim_{t_0 \rightarrow \infty} \int_0^{t_0} \partial_{t'} C_\kappa(t', \langle a_\alpha(\mathbf{r}) ; t \rangle) dt' \quad (6.37)$$

with the correlation functions

$$C_\eta(t) = \int d\Gamma \beta'_{3y} \cdot (1 - \mathcal{P}) e^{-\bar{\mathcal{L}}t} M_\eta, \quad (6.38)$$

$$C_\kappa(t) = \int d\Gamma \beta'_{3x} \cdot (1 - \mathcal{P}) e^{-\bar{\mathcal{L}}t} M_\kappa, \quad (6.39)$$

$$M_\eta \equiv \int d\mathbf{r}' x' \left( \frac{\delta \rho_{0\ell}}{\delta U_y(\mathbf{r}', t)} \right)_{\delta \langle a_\alpha ; t \rangle = 0}. \quad (6.40)$$

$$M_\kappa \equiv \int d\mathbf{r}' y' \left( \frac{\delta \rho_{0\ell}}{\delta U_y(\mathbf{r}', t)} \right)_{\delta \langle a_\alpha ; t \rangle = 0}. \quad (6.41)$$

This completes the formal derivation of the constitutive equations leading to the nonlinear Navier-Stokes equations, including expressions for the cooling rate, energy flux, and pressure tensor including contributions up through first order in the gradients of the hydrodynamic fields. These expressions are functions of the hydrodynamic fields to be determined by their detailed many-body analysis of the correlation functions.

## B. Green-Kubo expressions

To contrast the results here with those for an atomic fluid, it is instructive to focus on the Green-Kubo forms for the transport coefficients [3]. These are given by the second equalities of (6.22), (6.28), (6.29), (6.36), and (6.37); the first equalities are the corresponding Helfand forms [28]. For an atomic fluids there is no counter part to  $\omega_1$  and  $\mu$ . However, there are Green-Kubo expressions for the thermal conductivity and the two viscosities. For the discussion here only the thermal conductivity is considered, whose Green-Kubo expression is

$$\lambda(\langle a_\alpha(\mathbf{r}); t \rangle) = C_\lambda(0, \langle a_\alpha(\mathbf{r}); t \rangle) + \lim_{t_0 \rightarrow \infty} \int_0^{t_0} \partial_{t'} C_\lambda(t', \langle a_\alpha(\mathbf{r}); t \rangle) dt' \quad (6.42)$$

$$\partial_t C_\lambda(t) = \frac{1}{3} \int d\Gamma \beta'_2 \cdot (1 - \mathcal{P}) e^{-(\bar{\mathcal{L}} + K_{22})t} \mathbf{r}_\lambda, \quad (6.43)$$

$$\mathbf{r}_e = -(\bar{\mathcal{L}} + K_{22}) \mathbf{M}_e \quad (6.44)$$

In contrast the thermal conductivity for an atomic fluid is

$$\lambda(\langle a_\alpha(\mathbf{r}); t \rangle) \rightarrow \lim_{t_0 \rightarrow \infty} \int_0^{t_0} \partial_{t'} C_\lambda(t', \langle a_\alpha(\mathbf{r}); t \rangle) dt' \quad (6.45)$$

$$\partial_t C_\lambda(t) \rightarrow \frac{1}{3T^2} \int d\Gamma \beta'_2 \cdot (1 - \mathcal{P}) e^{-Lt} \beta'_2 \rho_e, \quad (6.46)$$

In this last expression  $\rho_e$  is the equilibrium Gibbs ensemble, and it is understood that  $\beta'_2$  is the microscopic expression for the energy flux for a dynamics with conservative forces, and  $L$  is the Liouville generator for the corresponding dynamics.

There are several similarities and differences between the granular and atomic fluid expressions [14]. The latter is the time integral of a energy flux - energy flux equilibrium time correlation function. The granular fluid is similar, with one of the fluxes the same but the other flux is generated from the local HCS state. Also, the generator for the dynamics in the granular case has two additional effects,  $L$  replaced by  $\bar{\mathcal{L}} + K_{22}$ , to represents homogeneous cooling of the reference state and its homogeneous response to perturbations. The projection orthogonal to the invariants of each dynamics  $(1 - \mathcal{P})$  occurs in both cases as a necessary condition for the long time limit of the time integral, and the corresponding existence of the normal state. Finally, the contribution from  $C_\lambda(0, \langle a_\alpha(\mathbf{r}); t \rangle)$  vanishes for a normal fluid but is non-zero for the granular fluid due to the non-conservative forces.

### C. Navier-Stokes hydrodynamic equations

In closing this section it is appropriate to record the results of substituting the Navier-Stokes constitutive equations, valid to first order in the gradients, into the exact macroscopic balance equations. This defines the Navier-Stokes hydrodynamic equations for a granular fluid

$$D_t m + m \nabla_{\mathbf{r}} \cdot \mathbf{U} = 0 \quad (6.47)$$

$$D_t e_0 + \omega_0 + \left( p + \omega_1 + \left( \frac{2}{3} \eta - \kappa \right) \nabla \cdot \mathbf{U} \right) \nabla \cdot \mathbf{U} - \eta (\partial_\alpha U_\beta + \partial_\beta U_\alpha) \partial_\alpha U_\beta - \nabla \cdot (\lambda \nabla T + \mu \nabla m) = 0, \quad (6.48)$$

$$D_t U_\alpha + m^{-1} \partial_\alpha \left( p - \left( \frac{2}{3} \eta + \kappa \right) \nabla \cdot \mathbf{U} \right) - m^{-1} \partial_\beta \eta (\partial_\alpha U_\beta + \partial_\beta U_\alpha) = 0. \quad (6.49)$$

For simplicity of notation,  $m \equiv \langle m(\mathbf{r}) ; t \rangle$  in these equations. They are a set of five nonlinear partial differential equations for the variables  $m$ ,  $e_0$ , and  $\mathbf{U}$ . They are a closed set of equations since  $\omega_0$ ,  $p$ , and the transport coefficients  $\omega_1$ ,  $\lambda$ ,  $\mu$ ,  $\eta$ , and  $\kappa$  are defined as functions of these variables. These definitions for the constitutive equations are the primary accomplishment of the statistical mechanical basis for the hydrodynamic equations. The form of (6.36)-(6.37) could have been guessed from the outset based on the macroscopic balance equations and fluid symmetry. The underlying basis in the microdynamics of the particles provides the necessary details for how the parameters of these equations must depend on the fields. Here only the formal definitions have been identified. It is only the first half of the problem of completing these equations, as the evaluation of these definitions poses a difficult many body problem. Still, without this first half, the starting point for that detailed analysis would not be possible. This is the case for atomic fluids as well.

## VII. FUTURE DIRECTIONS

The objective here has been to formulate the basis for a macroscopic description of granular fluids using the fundamental principles of nonequilibrium statistical mechanics. The analysis presented follows that for an atomic fluid. First, the exact macroscopic balance equations are identified. Next, their closure is linked to the concept of a normal state and corresponding normal solution to the Liouville equation. This defines the domain of hydrodynamics in its most general sense, both for atomic and granular fluids. The construction

of a normal solution is quite difficult in general, but can be accomplished for states with small gradients relative to locally homogeneous conditions. This gives the Navier-Stokes approximation described here.

Navier-Stokes hydrodynamics is applicable for most common states of atomic fluids, while deviations occur primarily for more complex polymeric molecular fluids. The latter have rheological properties corresponding to larger gradients relative to additional microscopic length and time scales. The construction of normal states in these cases is more difficult and is still at the semi-phenomenological stage [29]. Granular fluids provide a new motivation for renewed efforts to describe these more complex normal states. The reason is that even structurally simple granular fluids composed of spherically symmetric particles can exhibit rheology and other phenomena beyond the Navier-Stokes domain of validity [30, 31]. This is due to the cooling rate in the energy balance equation which provides a new internal time scale, that can set the size of hydrodynamic gradients beyond any control through boundary conditions. For example, new steady states are possible for granular fluids due to the balance of this internal cooling with external forcing. In many cases this implies that the hydrodynamic description required is beyond the Navier-Stokes domain. The understanding of constitutive equations in these cases is poor at this point. It is hoped that the formal structure described here will provide the appropriate basis for studies of these problems.

The context of hydrodynamics depends on the formation of a normal state from more complex conditions. Above this has been described qualitatively as a two stage process of rapid velocity relaxation in each cell to a state near the local HCS, followed by hydrodynamic relaxation through exchange of mass, energy, and momentum between the cells on a longer time scale. This separation of microscopic and hydrodynamic time scales is essential to the dominance of the hydrodynamic excitations over all others at large space and time scales. It is justified for atomic fluids since the hydrodynamic times are determined by the wavelength of the phenomena studied. As the system approaches homogeneity, these time scales become much larger than the microscopic excitations and hydrodynamics prevails at large times. However, there is an additional hydrodynamic time scale for granular fluids, the cooling rate, which is not set by the wavelength alone. It would seem that this additional time scale must be large as well, implying a weak cooling rate. This condition is too strong. What matters is the rate of the approach to the homogeneous state, not any dynamics of that final state. In the above derivation of hydrodynamics the final form for the solution to

the Liouville equation, eq. (6.16) or (6.17), has a dynamics generated by  $I\overline{\mathcal{L}} + K^T$  rather than simply that for the trajectories  $\overline{\mathcal{L}}$ . This is significant since the former has the additional compensation for the cooling and for the homogeneous perturbations of that cooling. Hence the approach to the time dependent normal state is determined only by the remaining non-hydrodynamic relaxation. The time scale for relaxation to the normal state is independent of the hydrodynamic time scales of that normal state. Quantitative verification of these concepts is another important future direction for research on a hydrodynamic description for granular fluids.

## VIII. ACKNOWLEDGMENTS

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## Appendix - Gradient expansion

In this Appendix the Liouville equation in the form (6.6) is written to first order in the gradients and solved. Also the invariants of the associated dynamics are identified.

Consider first the right side of (6.6) which can be written equivalently as

$$\begin{aligned}
& \int d\mathbf{r}' \frac{\delta \rho_{0\ell}}{\delta \langle a_\alpha(\mathbf{r}') ; t \rangle} \{ \nabla \cdot \langle \mathbf{b}_\alpha(\mathbf{r}) ; t \rangle + \delta_{\alpha 2} \langle w(\mathbf{r}) ; t \rangle \} - \bar{L} \rho_{0\ell} \\
&= - \int d\mathbf{r}' \frac{\delta \rho_{0\ell}}{\delta \langle a_\alpha(\mathbf{r}') ; t \rangle} \langle L a_\alpha(\mathbf{r}') ; t \rangle - \bar{L} \rho_{0\ell} \\
&= \int d\mathbf{r}' \frac{\delta \rho_{0\ell}}{\delta \langle a_\alpha(\mathbf{r}') ; t \rangle} \int d\Gamma a_\alpha(\mathbf{r}) \bar{L}(\rho_{0\ell} + \Delta) - \bar{L} \rho_{0\ell}
\end{aligned} \tag{1}$$

The first equality follows from (4.2) and (5.1). The first two terms are determined by the local HCS which can be expanded to first order in the gradients

$$\begin{aligned}
\rho_{0\ell} &= \rho_0(\langle a_\alpha(\mathbf{r}) ; t \rangle) + \int d\mathbf{r}' \left( \frac{\delta \rho_{0\ell}}{\delta \langle a_\alpha(\mathbf{r}') ; t \rangle} \right)_{\delta \langle a_\alpha ; t \rangle = 0} (\langle a_\alpha(\mathbf{r}') ; t \rangle - \langle a_\alpha(\mathbf{r}) ; t \rangle) + \dots \\
&= \rho_0(\langle a_\alpha(\mathbf{r}) ; t \rangle) + \mathbf{m}_\beta(\mathbf{r}, \langle a_\alpha(\mathbf{r}) ; t \rangle) \cdot \nabla \langle a_\beta(\mathbf{r}) ; t \rangle + \dots
\end{aligned} \tag{2}$$

The functional derivatives are

$$\begin{aligned}
\left( \frac{\delta \rho_{0\ell}}{\delta \langle a_\alpha(\mathbf{r}') ; t \rangle} \right)_{\delta \langle a_\alpha ; t \rangle = 0} &= \delta(\mathbf{r}' - \mathbf{r}) \left( \frac{\partial \rho_0(\langle a_\alpha(\mathbf{r}) ; t \rangle)}{\partial \langle a_\alpha(\mathbf{r}) ; t \rangle} + \frac{\partial \mathbf{m}_\beta(\mathbf{r}, \langle a_\alpha(\mathbf{r}) ; t \rangle)}{\partial \langle a_\alpha(\mathbf{r}) ; t \rangle} \cdot \nabla \langle a_\beta(\mathbf{r}) ; t \rangle \right) \\
&\quad + \mathbf{m}_\alpha(\mathbf{r}, \langle a_\alpha(\mathbf{r}) ; t \rangle) \cdot \nabla \delta(\mathbf{r}' - \mathbf{r}) + \dots
\end{aligned} \tag{3}$$

Here,

$$\mathbf{m}_\beta(\mathbf{r}, \langle a_\alpha(\mathbf{r}) ; t \rangle) \equiv \int d\mathbf{r}' \left( \frac{\delta \rho_{0\ell}}{\delta \langle a_\beta(\mathbf{r}') ; t \rangle} \right)_{\delta \langle a_\alpha ; t \rangle = 0} (\mathbf{r}' - \mathbf{r}), \tag{4}$$

and  $\rho_0(\langle a_\alpha(\mathbf{r}) ; t \rangle)$  is the actual HCS with its global density, energy, and momentum evaluated at the common values  $\langle a_\alpha(\mathbf{r}) ; t \rangle$ . It follows from (6.4) that the averages of  $a_\alpha(\mathbf{r})$  for  $\rho$ ,  $\rho_{0\ell}$ , and  $\rho_0$  are all the same. This in turn gives

$$\int d\Gamma a_\alpha(\mathbf{r}) \mathbf{m}_\beta = 0 = \int d\Gamma a_\alpha(\mathbf{r}) \Delta. \tag{5}$$

With these results and the fact that  $\Delta$  is of first order in the gradients, (1) to first order in the gradients becomes

$$\begin{aligned} & \int d\mathbf{r}' \frac{\delta \rho_{0\ell}}{\delta \langle a_\alpha(\mathbf{r}') ; t \rangle} \{ \nabla \cdot \langle \mathbf{b}_\alpha(\mathbf{r}) ; t \rangle + \delta_{\alpha 2} \langle w(\mathbf{r}) ; t \rangle \} - \bar{L} \rho_{0\ell} \\ & \rightarrow \bar{\mathcal{L}} \rho_0 - (1 - \mathcal{P}) (I \bar{\mathcal{L}} + K^T)_{\alpha\beta} \mathbf{m}_\beta \cdot \nabla \langle a_\alpha ; t \rangle + \mathcal{P} \bar{\mathcal{L}} \Delta \end{aligned} \quad (6)$$

The matrix  $K^T$  is the transpose of  $K$

$$K_{\alpha\beta} = \delta_{\alpha 2} \frac{\partial \omega(\langle a_\alpha(\mathbf{r}) ; t \rangle)}{\partial \langle a_\beta(\mathbf{r}) ; t \rangle}, \quad (7)$$

and  $I$  is the unit matrix. The generator  $\bar{\mathcal{L}}$  is the same as that of (3.12) with  $\omega \rightarrow \omega_0(\langle a_\alpha(\mathbf{r}) ; t \rangle)$  for the HCS evaluated at the common values  $\langle a_\alpha(\mathbf{r}) ; t \rangle$

$$\bar{\mathcal{L}} = -\omega_0(\langle a_\alpha(\mathbf{r}) ; t \rangle) \partial_{\langle e(\mathbf{r}) ; t \rangle} + \bar{L}. \quad (8)$$

Finally,  $\mathcal{P}$  is the projection operator

$$\mathcal{P}X = \frac{\partial \rho_0}{\partial \langle a_\alpha(\mathbf{r}) ; t \rangle} \int d\Gamma a_\alpha(\mathbf{r}) X. \quad (9)$$

The first term of (6) vanishes by definition of the HCS,  $\rho_0$ , confirming that the right side of the Liouville equation (6.6) is of first order in the gradients.

At this point, the Liouville equation (6.6) becomes

$$\partial_t \Delta - \int d\mathbf{r}' \frac{\delta \Delta}{\delta \langle a_2(\mathbf{r}') ; t \rangle} \omega_0(\langle a_\alpha(\mathbf{r}') ; t \rangle) + \mathcal{P} \bar{\mathcal{L}} \Delta = (1 - \mathcal{P}) \Upsilon'_\alpha \cdot \nabla \langle a_\alpha ; t \rangle, \quad (10)$$

$$\Upsilon'_\alpha \equiv - (I \bar{\mathcal{L}} + K^T)_{\alpha\beta} \mathbf{m}_\beta \quad (11)$$

This equation is still exact up through contributions of first order in the gradients. It has solutions of the form

$$\Delta(\Gamma, t | \langle a_\alpha(\mathbf{r}) ; t \rangle) = \mathbf{G}_\nu(\Gamma, t, \langle a_\alpha(\mathbf{r}) ; t \rangle) \cdot \nabla \langle a_\nu(\mathbf{r}) ; t \rangle, \quad (12)$$

Substitution into (10) gives the corresponding equation for  $\mathbf{G}_\nu$

$$\partial_t \mathbf{G}_\nu + (1 - \mathcal{P}) (I \bar{\mathcal{L}} + K^T)_{\nu\beta} \mathbf{G}_\beta = (1 - \mathcal{P}) \Upsilon'_\nu, \quad (13)$$

with the solution

$$\mathbf{G}_\nu(\Gamma, t, \langle a_\alpha(\mathbf{r}) ; t \rangle) = \int_0^t dt' \left( e^{-(1-\mathcal{P})(I \bar{\mathcal{L}} + K^T)t'} \right)_{\nu\beta} (1 - \mathcal{P}) \Upsilon'_\beta. \quad (14)$$

It is possible to add to (10) an arbitrary solution to the homogeneous equation corresponding to (13). As described in the text, this represents the dynamics of the first stage of rapid velocity relaxation to the local HCS. The interest here is in the second stage where possible formation of a normal solution occurs. Hence, it is simpler to choose that stage for initial conditions (initial local HCS).

Define the derivatives of the HCS by

$$\Psi_\beta(\Gamma, \langle a_\alpha(\mathbf{r}); t \rangle) \equiv \frac{\partial \rho_0}{\partial \langle a_\beta(\mathbf{r}); t \rangle}. \quad (15)$$

Then differentiate the equation for  $\rho_0$

$$\frac{\partial}{\partial \langle a_\beta(\mathbf{r}); t \rangle} \bar{\mathcal{L}} \rho_0 = 0, \quad (16)$$

to get

$$(I\bar{\mathcal{L}}_T + K^T)_{\nu\beta} \Psi_\beta = 0. \quad (17)$$

Since  $(I\bar{\mathcal{L}}_T + K^T)$  is the generator for the dynamics in (14) this shows that  $\Psi_\beta$  are the invariants of that dynamics.

The projection operator  $\mathcal{P}$  in (18) acts only on phase functions with translational invariance. In that case (9) simplifies to

$$\mathcal{P}X = \Psi_\beta \int d\Gamma A_\beta X, \quad A_\beta = V^{-1} \int d\mathbf{r} a_\beta(\mathbf{r}). \quad (18)$$

The first equality of (5) becomes  $\mathcal{P}\mathbf{m}_\beta = 0$ . This in turn gives

$$\mathbf{m}_\beta = (1 - \mathcal{P}) \mathbf{m}_\beta = (1 - \mathcal{P}) \mathbf{M}_\beta, \quad \mathbf{M}_\beta \equiv \int d\mathbf{r}' \left( \frac{\delta \rho_{0\ell}}{\delta \langle a_\alpha(\mathbf{r}'); t \rangle} \right)_{\delta \langle a_\alpha; t \rangle = 0} \mathbf{r}'. \quad (19)$$

Then  $(1 - \mathcal{P}) \Upsilon'_\alpha$  simplifies to

$$(1 - \mathcal{P}) \Upsilon'_\alpha = -(1 - \mathcal{P}) (I\bar{\mathcal{L}} + K^T)_{\alpha\beta} (1 - \mathcal{P}) \mathbf{M}_\beta \equiv (1 - \mathcal{P}) \Upsilon_\alpha \quad (20)$$

with

$$\Upsilon_\alpha = -(I\bar{\mathcal{L}} + K^T)_{\alpha\beta} \mathbf{M}_\beta. \quad (21)$$

Use has been made of the identity

$$(1 - \mathcal{P}) (I\bar{\mathcal{L}} + K^T) \mathcal{P} = 0. \quad (22)$$

This same identity leads to a simplification of the dynamics in (14)

$$e^{-(1-\mathcal{P})(I\bar{\mathcal{L}}+K^T)t'} (1 - \mathcal{P}) = (1 - \mathcal{P}) e^{-(I\bar{\mathcal{L}}+K^T)t'} (1 - \mathcal{P}). \quad (23)$$

In summary, the solution to the Liouville equation to first order in the gradients is

$$\begin{aligned}
\rho(\Gamma, t \mid \langle a_\alpha; t \rangle) = & \rho_0(\Gamma, \langle a_\alpha(\mathbf{r}); t \rangle) + (1 - \mathcal{P})(\mathbf{M}_\beta(\Gamma, \langle a_\alpha(\mathbf{r}); t \rangle) \\
& + \int_0^t dt' \left( e^{-(I\bar{\mathcal{L}} + K^T)t'} \right)_{\nu\beta} (1 - \mathcal{P}) \Upsilon_\beta(\Gamma, \langle a_\alpha(\mathbf{r}); t \rangle) \cdot \nabla \langle a_\nu(\mathbf{r}); t \rangle
\end{aligned} \tag{24}$$